Modeling Carbon Nanotube Electronic Devices

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Research is ongoing at Ames Research Center to characterize carbon nanotubes in order to exploit their remarkable properties for applications involving strong and lightweight composite materials and nanometer-scale electronic and electromechanical devices and sensors.

Discovered less than 10 years ago, carbon nanotubes are a form of elemental carbon that exhibits interesting electronic and mechanical properties. They can be visualized as resulting from rolling up a single layer of graphite (called a graphene sheet) to make a cylinder. Graphene sheets are hexagonal arrays of carbon atoms. They can be rolled up in a variety of directions (as denoted by two indices, e.g., (10,10), (12,8), and (17,0), which indicate how many steps up and across the array are taken to close the tube). The more interesting variety of nanotubes is *single-walled* (that is, they are a single cylinder), with diameters in the range of 1–3 nanometers and lengths of approximately 1 micron. Other nanotubes consist of concentric cylinders and are called *multi-walled.* Multi-walled nanotubes are observed with diameters up to 100 nanometers. Carbon nanotubes are produced in energetic environments, such as in carbon arcs and by laser ablation of graphite.

Depending on the way in which they are rolled up (called the helicity), carbon nanotubes can have metallic, semiconductor, or insulator properties. Metallic tubes could be used as a kind of molecular wire, and junctions between tubes of different helicity could operate as nano-scale diodes or transistors. Scientists at Ames are using computational chemistry, molecular modeling, and solid state physics techniques to study the electronic properties of hypothetical nanotube junctions. Experiments at Stanford University and elsewhere are under way to verify the results of this modeling study.

One example of this work is presented here. A perfect nanotube consists of only hexagonal rings of carbon atoms. If defects in the form of pentagonal and heptagonal rings are introduced into the hexagonal lattice, the tube will experience a change in helicity and either a change in diameter or a sharp bend. Some examples of bends are shown in the figure along with the indices of the tubes on either side of the junction and the bend angle (the amount of deviation from a straight tube). The pentagonal and heptagonal defects are denoted p and h. Although these junctions are created by modeling, actual tubes with these bend angles have been observed by transmission electron microscopy of nanotube samples.

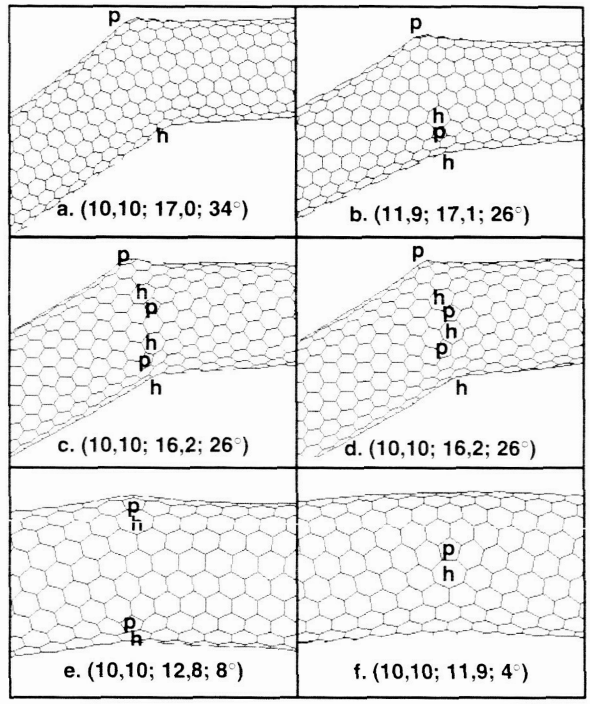

Fig. 1. Representative nanotube junctions.

The (10,10; 17,0) junction shown in part (a) of the figure is of particular interest because it connects a metallic and semiconducting tube. Calculations of the electron density of states at the junction indicate that this junction is electrically conducting and should function as a diode. This tube is nearly 100 times smaller than transistors in the most powerful microprocessor being made today.

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